

Non-unitary representations of the SU(2) algebra in the Dirac equation with a Coulomb potential

R. P. Martínez-y-Romero,* A. L. Salas-Brito

Laboratorio de Sistemas Dinámicos, Departamento de Ciencias Básicas, UAM-Azcapotzalco. Apartado Postal 21-726, Coyoacán 04000 DF, México.

E-mail: asb@hp9000a1.uam.mx

Jaime Saldaña-Vega

*Facultad de Ciencias, Universidad Nacional Autónoma de México,
Apartado Postal 50-542 México 04510 D. F.*

Abstract.

A novel realization of the classical SU(2) algebra is introduced for the Dirac relativistic hydrogen atom defining a set of operators that, besides, allow the factorization of the problem. An extra phase is needed as a new variable in order to define the algebra. We take advantage of the operators to solve the Dirac equation using algebraic methods. To accomplish this, a similar path to the one used in the angular momentum case is used; hence, the radial eigenfunctions calculated comprise non unitary representations of the algebra. One of the interesting properties of such non unitary representations is that they are not labeled by integer nor by half-integer numbers as happens in the usual angular momentum representation.

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* On sabbatical leave from Facultad de Ciencias UNAM,
e-mail: rodolfo@dirac.fciencias.unam.mx

I. Introduction

The unitary representations of groups and algebras are of a great interest in physics. We can mention the ubiquitous example of angular momentum or the $SU(2)$ algebra. In this instance, as it is well known, the representations are labeled by two real numbers j and m which may take only integer or half-integer values; the representations depend only on two parameters, θ and ϕ say, which are defined in the compact sets $[0, \pi]$ and $[0, 2\pi]$ respectively.¹ However, there are many other physically interesting groups or algebras which are not unitary. In such a case, the representations are not restricted to parameters defined in compact sets nor its generators are necessarily Hermitian, but they nevertheless can play an important role in physics. The Lorentz group being a very important example of a physically relevant non compact group whose algebra is not necessarily unitary.²

It is the purpose of this article to introduce a realization of the cyclic $SU(2)$ algebra in terms of non Hermitian operators and then to use these operators to factorize and solve the relativistic Dirac hydrogen atom. The solution is obtained using algebraic methods using the basic operators of the system, following a route parallel to the unitary compact case, but introducing an extra variable (found below to play the role of a phase) which is required in our approach.³

The use of algebraic techniques has been common for these sort of problems. For example, in the relativistic hydrogen atom à la Dirac one approach has been the use of shift operators;⁴ whereas in the non relativistic case a successful approach requires the use of ladder operators and the factorization method.⁵⁻⁶ Our approach is more akin to the introduction of ladder operators than to the shift operator method customarily used for this problem.⁴

The paper is organized as follows. In section II we introduce the equations of the problem and define our notation. In section III we construct the basic operators spanning the $SU(2)$ algebra as a useful tool for the problem. In section IV we define the inner product needed to investigate the properties of our basic operators. In section V some non unitary representations of the symmetry algebra are constructed as the radial eigenfunctions of the problem. We find that they are non compact representations that play an equivalent role to the spherical harmonics in the unitary case. In order to write such representations we find convenient to define a family of polynomials that are found to be the associated generalized Laguerre polynomials. In section VI, using algebraic methods and the operators defined in section II, we find the energy spectrum of the hydrogen

atom. In section VII we give our conclusions. In the Appendix, we list and plot the explicit expressions of the first 6 mentioned polynomials; they are explicitly related to the generalized associated Laguerre polynomials previously used by Davis for expressing the radial eigenfunctions of the hydrogen atom.⁷

II. The Dirac hydrogen atom

The symmetry algebra for the bound states of the non-relativistic hydrogen atom, even in the classical case, is well known to be the $SO(4)$,^{8,9} but in the relativistic case the situation is different as it is well known. The algebra associated with the symmetry of the radial part of the problem can be regarded as $SU(2)$ as occurs with the angular momentum. The beautiful thing is that we can then proceed to solve the relativistic hydrogen atom following a method that essentially parallels the calculation of eigenfunctions and eigenvalues of the angular momentum at the only expense of introducing an extra phase.

Let us begin with the Dirac Hamiltonian of the hydrogen atom

$$H_D = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta m - \frac{Ze^2}{r}, \quad (1)$$

where m is the mass of an electron and $\boldsymbol{\alpha}$ and β are the standard Dirac matrices¹⁰

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (2)$$

where the 1's and 0's stand, respectively, for 2×2 unit and zero matrices and the $\boldsymbol{\sigma}$ is the standard vector composed by the three Pauli matrices $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. Since the Hamiltonian (1) is invariant under rotations, the solutions of the problem can be written in the form

$$\psi(r, \theta, \phi) = \frac{1}{r} \begin{pmatrix} F(r)\mathcal{Y}_{jm}(\theta, \phi) \\ iG(r)\mathcal{Y}'_{jm}(\theta, \phi) \end{pmatrix}. \quad (3)$$

Where \mathcal{Y}_{jm} and \mathcal{Y}'_{jm} are spinor spherical harmonics of opposed parity. Parity is a good quantum number in the problem because the Coulomb potential is invariant under reflections; parity goes as $(-1)^l$ and, according to the triangle's rule of addition of momenta, the orbital angular momentum l is given by $l = j \pm \frac{1}{2}$. But, instead of working directly with parity, we prefer to introduce the quantum number ϵ defined by

$$\epsilon = \begin{cases} 1 & \text{If } l = j + \frac{1}{2}, \\ -1 & \text{If } l = j - \frac{1}{2}. \end{cases} \quad (4)$$

Thus $l = j + \frac{\epsilon}{2}$ in all cases; we also define $l' = j - \frac{\epsilon}{2}$. Accordingly, the spherical spinor \mathcal{Y}_{jm} depends on l whereas the spherical spinor \mathcal{Y}'_{jm} , which has an opposite parity, depends on l' . Writing the solutions in the form (3) completely solves the angular part of the problem.

Let us now address the radial part of the problem; we are interested in its bound states, then the quantity $k \equiv \sqrt{m^2 - E^2}$ is positive definite; furthermore, let us define

$$\zeta \equiv Ze^2, \quad \tau_j \equiv \epsilon(j + \frac{1}{2}), \quad \nu \equiv \sqrt{\frac{m-E}{m+E}}, \quad (5)$$

then, we can write the differential equations for the radial part of the problem, in terms of the dimensionless variable $\rho = kr$, as

$$\left(-\frac{d}{d\rho} + \frac{\tau_j}{\rho} \right) G(\rho) = \left(-\nu + \frac{\zeta}{\rho} \right) F(\rho), \quad (6)$$

and

$$\left(+\frac{d}{d\rho} + \frac{\tau_j}{\rho} \right) F(\rho) = \left(\nu^{-1} + \frac{\zeta}{\rho} \right) G(\rho); \quad (7)$$

these equations are to be regarded as the initial formulation of our problem.

The first thing we want to do is to show that Eqs. (6) and (7) can be rewritten using a set of three operators whose commutation relations define a SU(2) algebra. To this end, let us first introduce the new variable x through the relation (but please notice that this change is not required for any of the conclusions that follow, see the second remark below after Eq. (15))

$$\rho = e^x, \quad (8)$$

so x is defined in the open interval $(-\infty, \infty)$ and redefine the radial functions $F(\rho)$ and $G(\rho)$, introduced in equations (6) and (7), in the form

$$F(\rho(x)) = \sqrt{m+E} [\psi_-(x) + \psi_+(x)], \quad (9)$$

$$G(\rho(x)) = \sqrt{m-E} [\psi_-(x) - \psi_+(x)]. \quad (10)$$

In terms of the new functions $\psi_+(x)$ and $\psi_-(x)$, we thus arrive to the following set of equations for our problem

$$\left[\frac{d}{dx} + e^x - \frac{\zeta E}{\sqrt{m^2 - E^2}} \right] \psi_+(x) = \left(\frac{\zeta m}{\sqrt{m^2 - E^2}} - \tau_j \right) \psi_-(x), \quad (11)$$

and

$$- \left[\frac{d}{dx} - e^x + \frac{\zeta E}{\sqrt{m^2 - E^2}} \right] \psi_-(x) = \left(\frac{\zeta m}{\sqrt{m^2 - E^2}} + \tau_j \right) \psi_+(x). \quad (12)$$

This first-order system can be uncoupled multiplying by the left the first equation (Eq. (11)) times the operators that appear between square brackets in the second equation and, viceversa, by multiplying the second equation (Eq. (12)) times the operators that appear (between square brackets) in the first one. This procedure gives us the second order system

$$\left[\frac{d^2}{dx^2} + 2\mu e^x - e^{2x} - \frac{1}{4} \right] \psi_+(x) = \left(\tau_j^2 - \zeta^2 - \frac{1}{4} \right) \psi_+(x), \quad (13)$$

and

$$\left[\frac{d^2}{dx^2} + 2(\mu - 1)e^x - e^{2x} - \frac{1}{4} \right] \psi_-(x) = \left(\tau_j^2 - \zeta^2 - \frac{1}{4} \right) \psi_-(x), \quad (14)$$

where we have defined

$$\mu \equiv \frac{\zeta E}{\sqrt{m^2 - E^2}} + 1. \quad (15)$$

At this point there are several remarks that need to be done. First, in the next section the seemingly odd term $-1/4$ in Eqs. (13) and (14) is shown to be necessary to construct the algebra. Second, as we said before, the change of variable from ρ to x is not really necessary for any of the calculations in the article, however, we prefer to work in the x rather than in the ρ variable because this choice simplifies the appearance of some of the equations and, mainly, because it makes the inner product introduced in section III (in Eq. 33) look more familiar; but to make contact with the usual description we sometimes, at our convenience, revert to the variable ρ . As a third remark, notice that we can regard equations (13) and (14) as two eigenvalue equations where the common eigenvalue ω is given by

$$\omega = \tau_j^2 - \zeta^2 - \frac{1}{4} = j(j+1) - \zeta^2; \quad (16)$$

as it is obvious, we do not need to calculate ω because it follows directly from the radial symmetry of the problem and from the intensity of the interaction which is needed to set the scale. The fourth remark we want to do is that, as the minimum value of j is $1/2$, then $\omega \geq 0$ for at least $Z = 1, 2, \dots$ up to 118; for a discussion of the significance of this number see Ref. 4, page 236.

III. An operator algebra for the Dirac hydrogen atom

As the main purpose of this article is the construction of non unitary representations of the SU(2) algebra for the Dirac hydrogen atom,³ let us first introduce the operator

$$\Omega_3 \equiv -i \frac{\partial}{\partial \xi}, \quad (17)$$

depending exclusively on a new variable ξ , which is essentially an extra phase as must be clear in what follows, and the two operators

$$\Omega_{\pm} \equiv e^{\pm i\xi} \left(\frac{\partial}{\partial x} \mp e^x \mp i \frac{\partial}{\partial \xi} + \frac{1}{2} \right). \quad (18)$$

which depend both on ξ and on the transformed ‘radial’ variable x . These three operators satisfy the following algebraic relations

$$[\Omega_3, \Omega_{\pm}] = \pm \Omega_{\pm}, \quad (19)$$

and

$$[\Omega_+, \Omega_-] = 2\Omega_3. \quad (20)$$

We can alternatively define the two operators Ω_1 and Ω_2 as

$$\Omega_1 = \frac{1}{2} (\Omega_+ + \Omega_-), \quad \Omega_2 = \frac{1}{2i} (\Omega_+ - \Omega_-), \quad (21)$$

in terms of which the algebraic properties (19) and (20) read

$$[\Omega_i, \Omega_j] = i\epsilon_{ijk}\Omega_k, \quad i, j, k = 1, 2, 3. \quad (22)$$

It is now clear that the commutation relations (19) and (20) —or just (22) — correspond to an SU(2) algebra.^{1,3,8} To complete the discussion, we also need to introduce the Casimir operator of the algebra; let us consider the operator

$$\Omega^2 = \Omega_1^2 + \Omega_2^2 + \Omega_3^2, \quad (23)$$

we can easily show that (23) is indeed a Casimir for the algebra (19) and (20) (or (22))

$$[\Omega^2, \Omega_i] = 0. \quad \text{for } i = 1, 2, 3. \quad (24)$$

Here, as in the angular momentum case, we can regard Ω^2 as the square of $\mathbf{\Omega} = \Omega_1 \hat{\mathbf{i}} + \Omega_2 \hat{\mathbf{j}} + \Omega_3 \hat{\mathbf{k}}$. To obtain the explicit expression of Ω^2 , it is better to calculate first the product $\Omega_- \Omega_+$:

$$\Omega_- \Omega_+ = \frac{\partial^2}{\partial x^2} - e^{2x} - 2ie^x \frac{\partial}{\partial \xi} + i \frac{\partial}{\partial \xi} + \frac{\partial^2}{\partial \xi^2} - \frac{1}{4} \quad (25)$$

and obtain the Casimir operator from the relationship $\Omega^2 = \Omega_- \Omega_+ + \Omega_3(\Omega_3 - 1)$. We remark that we do not have a linear term in $\partial/\partial x$ in equation (22) because we choose the last constant in equation (18) precisely as $1/2$. We then easily conclude that the Casimir operator is given explicitly by

$$\Omega^2 = \frac{\partial^2}{\partial x^2} - e^{2x} - 2ie^x \frac{\partial}{\partial \xi} - \frac{1}{4}. \quad (26)$$

Although we are not restricted to a compact set of parameters anymore due to the presence of the variable x , in analogy with the conventions used for the *spherical harmonics* $Y_l^m(\theta, \phi)$, we label the simultaneous eigenfunctions of Ω^2 and Ω_3 as $V_\omega^\mu(x, \alpha)$; where the numbers ω are the eigenvalues of Ω^2 and the numbers μ are the eigenvalues of Ω_3 . Therefore, we write

$$\Omega_3 V_\omega^\mu(x, \xi) = \mu V_\omega^\mu(x, \xi) \quad (27)$$

and

$$\Omega^2 V_\omega^\mu(x, \xi) = \omega V_\omega^\mu(x, \xi); \quad (28)$$

we thus have

$$V_\omega^\mu(x, \xi) = e^{i\mu\xi} \mathcal{P}_\omega^\mu(x). \quad (29)$$

Where, again, we have used the angular momentum analogy to write the x functions as $\mathcal{P}_\omega^\mu(x)$, resembling the usual notation for the Legendre polynomials $P_l^m(\theta)$. In this equation it becomes clear the role of ξ as just an extra phase.

Notice that Eqs. (26) and (28) serve to establish the connection between the introduced operators of the SU(2) algebra and the radial part of the hydrogen atom problem, since applying the Casimir operator Ω^2 to $V_\omega^\mu(x, \xi)$ or to $V_\omega^{\mu-1}(x, \xi)$, reproduces Eqs. (13) and (14). Furthermore, comparison with these same equations tell us that

$$\psi_+(x) = \mathcal{P}_\omega^\mu(x), \quad (30)$$

$$\psi_-(x) = \mathcal{P}_\omega^{\mu-1}(x). \quad (31)$$

The operators Ω_\pm play the role of ladder operators for the problem; they move along the set of eigenfunctions changing the eigenvalue μ to the eigenvalue $\mu \pm 1$, in a completely analogous way to the case of the angular momentum algebra,

$$\Omega_\pm V_\omega^\mu(x, \xi) \propto V_\omega^{\mu \pm 1}(x, \xi), \quad (32)$$

the required proportionality constants are evaluated in section V (Eq. (52)).

IV. The inner product and related properties of the operators

To establish the properties of the Ω -operators and to construct the representations of the SU(2) algebra they span, we need a properly defined inner product. Here we cannot longer rely on the angular momentum analogy, since two of the parameters of the algebra we purport to construct are defined over the non-compact interval $(-\infty, \infty)$, making it completely different from the angular momentum. This situation implies that not all the generators of the algebra are to be Hermitian (indeed, Ω_3 is found to be Hermitian but Ω_1 and Ω_2 are found to be anti-Hermitian) and, as a consequence, that the corresponding group could not be unitary.

Let us consider the operation

$$(\phi, \psi) = \int_0^{2\pi} \frac{d\xi}{2\pi} \int_{-\infty}^{\infty} \phi^*(\xi, x) \psi(\xi, x) dx. \quad (33)$$

It is easy to show that Eq. (33) defines an inner product, since, as it is not difficult to prove, it satisfies the three basic properties:

- i) If $\psi(x) = 0$, then $(\psi, \psi) = 0$.
- ii) If $\psi(x) \neq 0$, then $(\psi, \psi) \geq 0$.
- iii) If c is any complex number, then $(\psi, c\phi) = c(\psi, \phi)$ and $(c\psi, \phi) = c^*(\psi, \phi)$.

To study the behavior of the generators of the algebra in terms of the inner product (33), we consider a certain function $\psi(x, \xi)$ associated to a certain fixed value μ_0 . We define the elements of the associated Hilbert space H_{μ_0} with functions of the form

$$\psi(x, \xi) = e^{i(\mu_0 + m - n)\xi} \mathcal{F}(x), \quad (34)$$

where m and n are integer numbers and $\mathcal{F}(x)$ is a well behaved function depending only on x . As we exhibit in section V, this is actually the general form of the functions inhabiting the Hilbert space of our problem.

With the help of the inner product (33), we can establish the properties of the Ω_a ($a = 1, 2, 3$) operators. Let us consider first Ω_3 , in this case the important product is

$$(\psi', \Omega_3 \psi) = \delta_{m'-n', m-n} (\mu_0 + m - n) \int_{-\infty}^{\infty} \mathcal{F}^*(x) \mathcal{F}(x) dx; \quad (35)$$

this last equation, due to the presence of the Kronecker delta, can be written as

$$\int_0^{2\pi} \frac{d\xi}{2\pi} \int_{-\infty}^{\infty} \left[i \frac{\partial}{\partial \xi} e^{-i(\mu_0 + m' - n')\xi} \right] e^{-i(\mu_0 + m - n)\xi} \mathcal{F}^*(x) \mathcal{F}(x) dx, \quad (36)$$

and this is precisely $(\Omega_3 \psi', \psi)$. We have in this way proved that Ω_3 is an Hermitian operator:

$$\Omega_3^\dagger = \Omega_3. \quad (37)$$

To study the operators Ω_\pm , let us first consider Ω_+ and evaluate the product

$$\begin{aligned} (\psi', \Omega_+ \psi) &= \int_0^{2\pi} \frac{d\xi}{2\pi} \int_{-\infty}^{\infty} e^{-i(\mu_0 + m' - n')\xi} \mathcal{F}^*(x) dx \\ &\quad e^{i\xi} \left(\frac{\partial}{\partial x} - e^x - i \frac{\partial}{\partial \xi} + \frac{1}{2} \right) e^{i(\mu_0 + m - n)\xi} \mathcal{F}(x) dx. \end{aligned} \quad (38)$$

To analyse this integral, it is simpler to split it in two parts. Let us consider first the $e^{i\xi}(-\partial/\partial\xi + 1/2)$ part; its contribution to the inner product (38) is

$$\left(\mu_0 + m - n + \frac{1}{2} \right) \delta_{m'-n', m-n+1} \int_{-\infty}^{\infty} \mathcal{F}^*(x) \mathcal{F}(x) dx, \quad (39)$$

this expression can be written as

$$-\int_0^{2\pi} \frac{d\xi}{2\pi} \left[e^{-i\xi} \left(i\frac{\partial}{\partial\xi} + \frac{1}{2} \right) e^{i(\mu_0+m'-n')\xi} \mathcal{F}(x) \right]^\dagger e^{i(\mu_0+m-n)\xi} \mathcal{F}(x) dx. \quad (40)$$

We now take care of the contribution of the term $e^{i\xi}(\partial/\partial\xi - e^x)$. After a partial integration this contribution becomes

$$\delta_{m'-n'-1,m-n} \int_{-\infty}^{\infty} \left[-\left(\frac{\partial}{\partial x} + e^x \right) \mathcal{F}(x) \right]^\dagger \mathcal{F}(x) dx. \quad (41)$$

Taking together the two previous results, it is easy to see that the operator complies with $\Omega_+^\dagger = -\Omega_-$. A similar calculation establish the analogous property $\Omega_-^\dagger = -\Omega_+$. Therefore, we have established that

$$\Omega_\pm^\dagger = -\Omega_\mp. \quad (42)$$

We have proved that not all the operators are Hermitian thence arriving to the anticipated results: First, we showed that the operator Ω_3 is indeed Hermitian, as a consequence we expect the range of the only parameter it depends on, ξ , to be compact; this is certainly the case since $\xi \in [0, 2\pi]$, a compact set. The other two operators Ω_1 and Ω_2 depend upon x , a variable defined over the non compact set $(-\infty, \infty)$, but here such operators are anti-Hermitian

$$\Omega_a^\dagger = -\Omega_a, \quad a = 1, 2 \quad (43)$$

as it is easy to show from Eqs. (21) and (42).

V. Representations of the SU(2) algebra (radial eigenfunctions of the problem).

With the inner product defined in the previous section, we are in the position of introducing a complete orthogonal basis of simultaneous eigenfunctions for Ω^2 and Ω_3 which accordingly must carry a representation of the algebra—and, besides, they solve our radial eigenvalue problem (Eqs. (6) and (7)). We have decided to choose the commuting operators in similar fashion to the standard SU(2) case. Let us define then

$$V_\omega^\mu(x, \xi) \equiv |\omega \mu >, \quad (44)$$

where the kets $|\omega \mu\rangle$ are both assumed orthogonal and normalized respect the inner product (33)

$$\langle \omega' \mu' | \omega \mu \rangle = \delta_{\omega, \omega'} \delta_{\mu, \mu'}. \quad (45)$$

Now, as Ω_1 and Ω_2 are not Hermitian, the Casimir operator Ω^2 defined in (23) is not necessarily positive definite, we can nevertheless introduce a positive definite operator as

$$\boldsymbol{\Omega}^\dagger \cdot \boldsymbol{\Omega} = -\Omega_1^2 - \Omega_2^2 + \Omega_3^2 = 2\Omega_3^2 - \Omega^2; \quad (46)$$

the positivity of this operator allows us to show that

$$2\mu^2 \geq \omega, \quad (47)$$

that is, $|\mu|$ is bounded by below. As a consequence, there must exist a minimum value for $|\mu|$, let us say $\lambda \equiv |\mu|_{\min}$. We also know the that the ket $|\omega \lambda\rangle$ is annihilated by Ω_- or, equivalently, that $\Omega_+ \Omega_- |\omega \lambda\rangle = 0$; so

$$\omega - \lambda^2 - \lambda = 0 \quad \text{or} \quad \omega = \lambda(\lambda - 1). \quad (48)$$

Given equation (47), let us introduce a slight change in notation, writing λ instead of ω in the eigenfunctions $\mathcal{P}_\omega^\mu(x)$ of Eq. (29), that is, $\mathcal{P}_\omega^\mu(x)$ is to be replaced by $\mathcal{P}_\lambda^\mu(x)$. Furthermore, as λ has to be positive and since $\omega = \tau_j^2 - \zeta^2 - 1/4$, we find that the minimum $|\mu|$ -value is

$$|\mu|_{\min} \equiv \lambda = s + \frac{1}{2}, \quad (49)$$

where we have defined

$$s \equiv +\sqrt{\tau_j^2 - \zeta^2} = \sqrt{(j + 1/2)^2 - \zeta^2}. \quad (50)$$

Notice that s is a real quantity for $Z = 1, 2, 3, \dots, 137$.

However, the most important conclusion we can draw from Eqs. (49) and (50), is that λ no longer has to be an integer or half-integer number, as necessarily happens in the unitary compact angular momentum case. We may see that this result is a direct consequence of both Ω_1 and Ω_2 not being Hermitian operators. So the operators introduced for the SU(2) algebra associated with the Dirac hydrogen atom lead naturally to non unitary representations labeled by real numbers, or, at least, not necessarily integer nor half-integer ones.

For constructing the functions comprising the representations, let us introduce the constants C_μ^\pm as follows (compare with Eq. (32))

$$\Omega_\pm |\omega \mu > = C_\mu^\pm |\omega \mu \pm 1 >; \quad (51)$$

these constants can be explicitly evaluated from $\langle \omega \mu | \Omega_+ \Omega_- | \omega \mu \rangle = C_\mu^- C_{\mu-1}^+$ and from $(C_{\mu-1}^+)^* = -C_\mu^-$; if we further assume these constants to be real, we easily get

$$C_\mu^\pm = \pm \sqrt{\mu(\mu \pm 1) - \lambda(\lambda - 1)}, \quad (52)$$

a result with a slightly different form than in the analogous angular momentum case.^{4,8}

The ground state of the hydrogen atom, can be obtained from the equation $\Omega_- |\lambda \lambda > = 0$ for the positive set of eigenvalues. Such equation becomes

$$e^{-i\xi} \left(\frac{\partial}{\partial x} + e^x - \lambda + \frac{1}{2} \right) e^{i\lambda\xi} \mathcal{P}_\lambda^\lambda(x) = 0. \quad (53)$$

whose solution is

$$\mathcal{P}_\lambda^\lambda(x) = d_\lambda e^{sx} \exp(-e^x) = d_\lambda e^{(\lambda-1/2)x} \exp(-e^x), \quad (54)$$

where

$$d_\lambda \equiv \frac{2^{(\lambda-1/2)}}{\sqrt{\Gamma(2\lambda-1)}} \quad (55)$$

is a normalization constant and $\Gamma(y)$ stands for the Euler-gamma function. Since λ is the lowest eigenvalue, in this instance we should have

$$\psi_+(x) = \mathcal{P}_\lambda^\lambda(x), \quad (56)$$

and

$$\psi_-(x) = 0. \quad (57)$$

In terms of the radial variable ρ , we can see from Eqs. (9) and (10) that the ground state solutions are

$$F(\rho) = \sqrt{\frac{(m+E)}{2m(\lambda-1/2)}} \rho^s e^{-\rho}, \quad (58)$$

and

$$G(\rho) = -\sqrt{\frac{(m-E)}{2m(\lambda-1/2)}}\rho^s e^{-\rho}. \quad (59)$$

normalized in the sense

$$\int_0^\infty (|F(\rho)|^2 + |G(\rho)|^2) d\rho = 1. \quad (60)$$

We can also see that in the case of negative eigenvalues the solutions behave as $\sim \rho^s e^\rho$, giving divergent behavior as $\rho \rightarrow \infty$. This behavior makes the negative energy solutions not square integrable; therefore, we have to discard them if we want to describe physically realizable states.^{2,3,10}

The excited states can be obtained, as we do in the appendix, by applying successively Ω_+ to the ground state $|\lambda\lambda\rangle$, as it is customarily done for the spherical harmonics. The result involves the functions $\mathcal{P}_\lambda^\mu(x)$ introduced by Eqs. (29) and (34). The $\mathcal{P}_\lambda^\mu(x)$ are polynomials multiplied by the weight factor $W(\rho) = \rho^{\lambda-1/2} e^{-\rho}$. This weight factor assures that the behavior of the big and the small components of the spinor are regular both at the origin as well as $\rho \rightarrow \infty$. As illustration of the solutions discussed here, we quote in the Appendix the first few cases of $\mathcal{P}_\lambda^{\lambda+p}(x)$, for $p = 0, \dots, 5$, there we also plot these polynomial part of the functions (*i. e.* we plot $\mathcal{P}_\lambda^\mu(x)$ without the weight factors) for the first 5 excited energy levels. Notice that the polynomial part in the eigenfunction $\mathcal{P}_\lambda^{\lambda+p}(x)$ is always of order p .

The matrix representations of the Ω_a , $a = 1, 2, 3$, for $\lambda = s + 1/2 + p$, $p = 0, 1, 2, 3, \dots$, are constructed from equations (27), (28), (51) and (52). In contrast with the standard SU(2) case, here the representations are non Hermitian and infinite dimensional for each λ , excepting for Ω_3 . The matrix elements of the operator Ω_3 , including the negative eigenvalue series, are given by

$$\langle \omega\mu | \Omega_3 | \omega\mu' \rangle = \mu \delta_{\mu\mu'}, \quad (61)$$

where $\mu = \pm(\lambda + p)$, $p = 0, 1, 2, \dots$; therefore, its trace vanishes and the determinant of any element of the corresponding group with the form $\exp(i\Omega_3)\xi$, is always 1.

For the other two operators the only non-vanishing matrix elements are

$$\langle \omega\mu | \Omega_1 | \omega\mu \pm 1 \rangle = \mp \frac{1}{2} \sqrt{\mu(\mu \pm 1) - \lambda(\lambda - 1)}, \quad (62)$$

$$\langle \omega\mu|\Omega_2|\omega\mu\pm 1\rangle = -\frac{i}{2}\sqrt{\mu(\mu\pm 1) - \lambda(\lambda-1)}, \quad (63)$$

This means again that the trace of both Ω_1 and Ω_2 vanish. Notice also that the determinant of a group element generated by Ω_1 or Ω_2 is 1 only for a purely imaginary parameter.

VI. The energy spectrum.

We can now evaluate the bound energy spectrum for the problem. As we mentioned in section V, the bound state energy spectrum comprises only the positive series eigenvalues.^{2,10} Let us first express the energy in terms of the eigenvalue μ from Eq. (15)

$$E = m \left[1 + \frac{\zeta^2}{(\mu - 1/2)^2} \right]^{-1/2}. \quad (64)$$

then, for the case of positive eigenvalues —the only ones with physically appropriate eigenfunctions— we have that $\mu = \lambda + p$, where p is an non negative integer $p = 0, 1, 2, \dots$, or, equivalently, that $\mu - 1/2 = s + p$. This gives precisely the energy spectrum of the relativistic hydrogen atom. To rewrite our result in a more familiar form, we need only to define the principal quantum number n and the auxiliary quantity ϵ_j as follows

$$n = j + \frac{1}{2} + p, \quad (65)$$

$$\epsilon_j = n - s - p = j + \frac{1}{2} - s; \quad (66)$$

we then finally conclude that $\mu - 1/2 = s + p = n - \epsilon_j$, which gives precisely the well-known energy spectrum.¹⁰

VII. Concluding remarks.

In summary, we have constructed an SU(2) algebra for the hydrogen atom in the Dirac formulation, introducing the Hermitian operator Ω_3 and the anti-Hermitian operators Ω_1 and Ω_2 . The result of all of this, is that the representations are labelled by numbers λ which are neither integers nor half-integers as in the case of the more familiar unitary representations. Nevertheless, the algebra introduced predicts precisely the energy eigenvalues and eigenfunctions of the Dirac hydrogen atom. One of the most noteworthy features of the representations reported here is the mixing of a spinorial angular momentum character, implying an equally spaced spectrum, with the energy requirements of

the problem—requiring a differently spaced spectrum; the interplay of these two spectral requirements is basically reflected in the fact that the eigenvalues associated with Eqs. (13) and (14) follows from both the generic radial symmetry and the specific features of the interaction in the Dirac equation (1). From Eq. (15) it also follows that in the limit of vanishing interaction, *i.e.* $\zeta \rightarrow 0$, our representations collapse and, in this special case, $\mu = 1$ always. Such behavior is precisely as expected because there is no longer any restriction over the eigenvalues and thus the spectrum becomes continuous, corresponding to a free Dirac particle. The operator algebra we introduced allows an essentially algebraic solutiond of Dirac hydrogen atom which may have various applications.^{3,4,6}

It is to be noted also the possible connections that our formulation may have with systems with hidden supersymmetric properties,^{13–16} as we will discuss in a forthcoming article. The energy spectrum of the problem has some peculiarities which also appear in the spectrum of a Dirac oscillator;^{14–15,17} in particular the equally spaced energy solutios for $\psi_+(x)$ and $\psi_-(x)$ resemble, respectively, the behavior of big and the small components of the aforementioned system. As a result of this resemblance, we are studying the hidden supersymmetric properties and the superconformal algebra, in the sense of Refs. 15 and 18, associated with this problem. The similitude of Eqs. (13) and (14) with the corresponding ones for a Morse oscillator should be also noticed.⁶

It is worth pinpointing that we are forced to introduce the new variable ξ in order to define the algebra; in terms of the solutions of the Dirac equation, ξ just plays the role of a phase. To exemplify, when we perform a “rotation” using Ω_3 , the big component changes from $F(x) \propto [\psi_-(x) + \psi_+(x)]$ to $F(x) \propto [e^{i(\mu-1)\xi}\psi_-(x) + e^{i\mu\xi}\psi_+(x)] = e^{i\mu\xi}[e^{-i\xi\psi_-(x)+\psi_+(x)}]$. The phase $e^{i\mu\xi}$ does not play any observable role, but the term $e^{-i\xi}$ changes the relative phase between the $\psi_+(x)$ and the $\psi_-(x)$ components of the eigenfunction and, in consequence, changes the radial function $F(\rho)$ itself although the energy spectrum is still invariant under such transformation; this is a consequence of the fact that $|\omega \mu >$ and $\Omega_3|\omega \mu >$ both correspond to the same eigenvalue μ . In a way, this resembles what happens when there are superselection rules in a system.^{19–21}

To finalize, let us comment that it is not widely known that the radial eigenfunctions of the Dirac hydrogen atom can be expressed in terms of generalized associated Laguerre polynomials, as was realized by Davis a long time ago.^{7,11} These polynomials, which are a generalization to non integral indices of the usual associated Laguerre polynomials, are defined as⁷

$$\mathcal{L}_p^\alpha(x) = \frac{\Gamma(\alpha + p + 1)}{n! \Gamma(\alpha + 1)} {}_1F_1(-p; \alpha + 1; x) \quad (67)$$

where $\Gamma(x)$ is again the Euler gamma function, p is a positive integer, and the ${}_1F_1(-p, \alpha+1; x)$ stands for the confluent hypergeometric function —having one of their arguments negative, the hypergeometric function reduces to a polynomial.¹² The polynomial representation of the radial eigenfunctions introduced here is related to that used by Davis in Eqs. (A8) and (A9) of the Appendix.

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Appendix

The purpose of this Appendix is to illustrate the behavior of the first few polynomials associated to the radial eigenfunction of the hydrogen atom in the base $|\lambda \mu\rangle$ and to relate this description to the old but little known results of Davis.^{7,11} We explicitly calculate the first 6 functions of the positive eigenvalue series, such functions are always of the form the weight factor $W(\rho)$ times a polynomial; the weight factor is $W(\rho) = \rho^s e^{-\rho}$. The polynomials are plotted in Figure 1. The radial eigenfunctions are essentially generated from the basic relationship $\Omega_+ |\omega \mu\rangle = C_\mu^+ |\omega \mu + 1\rangle$. In the ρ variable, the first equation in the series can be written as

$$e^{+i\xi} \left(\rho \frac{\partial}{\partial \rho} - \rho - i \frac{\partial}{\partial \xi} + \frac{1}{2} \right) e^{i\mu\xi} \mathcal{P}_\lambda^\lambda(\rho) = C_\mu^+ e^{i(\mu+1)\xi} \mathcal{P}_\lambda^{\lambda+1}(\rho) \quad (A1)$$

which is just the first term in the whole ascending series $\mathcal{P}_\lambda^{\lambda+p}(\rho) = \Omega_+^p \mathcal{P}_\lambda^\lambda(\rho)$ used to recursively calculate (A2–A7). Note that the polynomial part of the function $\mathcal{P}_\lambda^{\lambda+p}(x)$ is always of the form $\sum_{i=0}^p C_i(\lambda) \rho^i$, where $C_i(\lambda)$ is also an order $(p - i)$ polynomial in λ .

Starting with $\mu = \lambda$, the first few functions in the positive series are then given by

$$\mathcal{P}_\lambda^\lambda(\rho) = W(\rho), \quad (A2)$$

$$\mathcal{P}_\lambda^{\lambda+1}(\rho) = \sqrt{\frac{2}{\lambda}}(\lambda - \rho)W(\rho), \quad (A3)$$

$$\mathcal{P}_\lambda^{\lambda+2}(\rho) = \frac{W(\rho)}{\sqrt{2\lambda(\lambda+1/2)}}[2\rho^2 - (2\lambda+1)(2\rho-\lambda)], \quad (A4)$$

$$\begin{aligned} \mathcal{P}_\lambda^{\lambda+3}(\rho) &= \frac{W(\rho)}{\sqrt{3\lambda(\lambda+1/2)(\lambda+1)}}[-2\rho^3 + 6\rho^2(\lambda+1) - 3\rho(2\lambda^2 + 3\lambda + 1) \\ &\quad + \lambda(2\lambda^2 + 3\lambda + 1)], \end{aligned} \quad A(5)$$

$$\begin{aligned} \mathcal{P}_\lambda^{\lambda+4}(\rho) &= \sqrt{\frac{2}{3}} \frac{W(\rho)}{\sqrt{\lambda(\lambda+1/2)(\lambda+1)(\lambda+3/2)}}[\rho^4 - 2(3+2\lambda)\rho^3 + 3(3+5\lambda+2\lambda^2)\rho^2 \\ &\quad - (3+11\lambda+12\lambda^2+4\lambda^3)\rho + (\lambda^3+3\lambda^2+\frac{11}{4}\lambda+\frac{3}{4})\lambda], \end{aligned} \quad (A6)$$

$$\begin{aligned} \mathcal{P}_\lambda^{\lambda+5}(\rho) &= \frac{W(\rho)}{\sqrt{15\lambda(\lambda+1/2)(\lambda+1)(\lambda+3/2)(\lambda+2)}}[-\rho^5 + (5\lambda+\frac{29}{2})\rho^4 \\ &\quad - (10\lambda^2+51\lambda+54)\rho^3 + (10\lambda^3+66\lambda^2+\frac{235}{2}\lambda+\frac{123}{2})\rho^2 \\ &\quad - (5\lambda^4+37\lambda^3+\frac{319}{4}\lambda^2+\frac{257}{4}\lambda+\frac{33}{2})\rho + \lambda^5 + \frac{15}{2}\lambda^4 + \frac{65}{4}\lambda^3 \\ &\quad + \frac{105}{8}\lambda^2 + \frac{27}{8}\lambda]. \end{aligned} \quad (A7)$$

The relationship to these polynomials to those used by Davis can be seen from Eqs. (13) and (14), putting $\rho = \exp x$ and introducing the function $v(\rho)$ according to $\psi_+ \equiv \rho^s \exp(-\rho) v(\rho)$, and finally using $\mathcal{L}(\rho) \equiv v(\rho/2)$, to get

$$\rho \frac{d^2 \mathcal{L}}{d\rho^2} + [(2s+1) - \rho] \frac{d\mathcal{L}}{d\rho} + \left[\frac{(s^2 + \zeta^2 - \tau_j^2)}{\rho} + (\mu - s - 1/2) \right] \mathcal{L} = 0, \quad (A8)$$

where $\mu = s + 1/2 + p$. This equation can be regarded as a generalization to non integer index of the usual associated Laguerre differential equation. The equation corresponding to ψ_- can be obtained in analogous fashion. This equation reduces to the one used by Davis if and only if $s^2 = \tau_j^2 - \zeta^2$, a result which just recovers the definition in Eq. (50). Now we can give the explicit relationship between our representation of the radial eigenfunctions to that used by Davis as

$$\begin{aligned} \psi_+(\rho) &= \mathcal{P}_{s+1/2}^{s+1/2+p}(\rho) = \rho^s \exp(-\rho) \mathcal{L}_p^{2s}(2\rho), \\ \psi_-(\rho) &= \mathcal{P}_{s+1/2}^{s-1/2+p}(\rho) = \rho^s \exp(-\rho) \mathcal{L}_{p-1}^{2s}(2\rho) \end{aligned} \quad (A9)$$

save for normalization factors (unimportant for the point at hand) where $s = \lambda - 1/2$, and where the generalized associated Laguerre polynomials used by Davis are defined in Eq. (67).

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Figure Caption

Figure 1

We show the graph of the first polynomials $\mathcal{P}_\lambda^{\lambda+p}(\rho)/W(\rho)$, for $p = 1, 2, 3, 4, 5$, $Z = 1$ and $j = 1/2$. Notice the similarity of the behavior of all polynomials near the origin.

